Cyclohexane 110-82-7 | DTXSID4021923

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 129 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.86e-01

Confidence level: 7.99e-01

Nearest Neighbors from the Training Set

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Toluene

Measured: 117 Predicted: 87.4

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m-Xylene

Measured: 178 Predicted: 246 Image not found

ortho-Xylene Measured: 178

Predicted: 249

Image not found

Benzene

Measured: 56.2 Predicted: 50.5

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Ethylbenzene Measured: 170 Predicted: 271